ORGANIC CHEMISTRY - NOMENCLATURE

ORG.NOM.1

Organic chemistry is the chemistry of the **compounds of carbon.**

The misleading name "organic" is a relic of the days when chemical compounds were divided into two classes, inorganic and organic, depending upon where they had come from. Inorganic compounds were those obtained from minerals; organic compounds were those obtained from vegetable or animal sources, that is, from material produced by living organisms. Indeed, until about 1850 many chemists believed that organic compounds **must** have their origin in living organisms, and consequently could never be synthesized from inorganic material.

These compounds from organic sources had this in common: they all contained the element carbon. Even after it had become clear that these compounds did not have to come from living sources but could be made in the laboratory, it was convenient to keep the name **organic** to describe them and compounds like them. The division between inorganic and organic compounds has been retained to this day.

Aliphatic and Aromatic Compounds

Chemists have found it useful to divide all organic compounds into two broad classes: **aliphatic** compounds and **aromatic** compounds. The original meanings of the words "aliphatic" (fatty) and "aromatic" (fragrant) no longer have any significance.

Aliphatic compounds are open-chain compounds and those cyclic compounds that resemble the open-chain compounds. Aromatic compounds are benzene and compounds that resemble benzene in chemical behaviour. Benzene has the molecular formula C_6H_6. The carbon atoms are arranged in a closed hexagonal ring with alternating single and double bonds between adjacent carbon atoms. A more detailed description of benzene will follow.

THE COMMON NAMES OF SIMPLE ORGANIC COMPOUNDS

Saturated Aliphatic Hydrocarbons

Introduction: A hydrocarbon is a molecule made up of carbon atoms, hydrogen atoms and no other atoms.

1-1 In a hydrocarbon with n carbon atoms, the maximum number of hydrogen atoms is found to be given by the formula

maximum number of H atoms = $2n + 2$

If a hydrocarbon contains only one carbon atom, then $(2 \times 1) + 2$ or _____ is the _____ number of hydrogen atoms.

1-2 A hydrocarbon with the maximum number of hydrogen atoms is called an **alkane.**

Methane, or marsh gas, is an alkane. Its formula is CH_4 (one carbon, four hydrogens).

Ethane is an alkane; it has two carbon atoms, so its formula is C_2H___.

1-3 Propane is an alkane with three carbons; its formula is _____.

1-4 A hydrocarbon with the formula C_4H_{10} belongs to the class of _____ because it contains the _____ number of hydrogen atoms, given by the formula C_nH_____.

1-5 When we reach alkanes with four or more carbon atoms, we find that more than one compound has a given formula. Thus two different chemicals with four carbons and belonging to the alkanes exist. Both have the formula _____ .

1-6 In the one case, the four carbons are in a chain, C-C-C-C, whereas, in the other, only three are in a chain, the fourth being attached to the center of the chain, C-C-C. Carbon has a valence of 4 and

```
    |
    C
```

hydrogen is monovalent; a carbon atom forms four bonds with other atoms and hydrogen can only link to one other atom by one bond. When we attach hydrogen atoms to all the unused carbon valences, the four carbon chain formula can be represented as

```
      H H H H
      | | | |
    H-C-C-C-C-H
      | | | |
      H H H H
```

This is often called normal butane and written n-butane. If we attach all the hydrogens to the branched butane C-C-C (commonly called isobutane)

```
    |
    C
```

the corresponding formula would look like this:

1-7 Note: These extended formulas showing which atoms are attached to each other, are called structural formulas. The simpler formulas, such as C_4H_{10}, which merely show the total number of atoms of each element in the molecule are called molecular formulas.

Isobutane and n-butane are spoken of as isomers (from the Greek isos, equal, and meros, parts). Isomers are physically and/or chemically different substances with the same molecular formula.

The word butane is derived from the word butter. The unpleasant odour of rancid butter is due to an acid (butyric acid) containing four carbon atoms.

Now we have seen that there exist one methane (CH_4), one ethane (C_2H_6), and one propane (C_3H_8), but two substances with formula C_4H_{10}, whose carbon "skeletons" were C-C-C-C (n-butane) and C-C-C

```
    |
    C
```

(isobutane) respectively.

The reason for the two butanes is the presence of two different kinds of carbon atoms in propane (C-C-C): The propane molecule contains two identical end carbon atoms each directly attached to one carbon atom, and a middle carbon directly attached to two carbons.

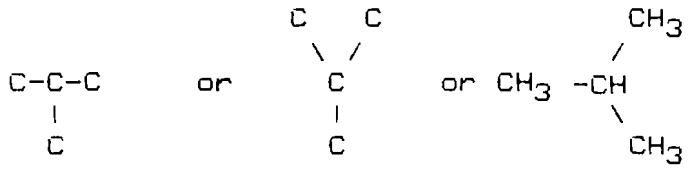
We define a **primary** (1°) carbon as a carbon attached to one or no other carbon atoms; a **secondary** (_____°) carbon as one attached to two other carbons, and a _____ (_____°) carbon as one attached to three other carbons.

1-8 A quaternary (4°) carbon is one utilizing all _____ of its bonds in attachments to other (number) _____ atoms. (element)

1-9 Thus propane (C-C-C) has _____ primary carbon atoms and _____ secondary carbon(s).

1-10 If we attach a carbon atom to a primary carbon of propane, we obtain n-butane, C-C-C-C, which has _____ primary carbon and _____ secondary carbons.

1-11 If, however, the fourth carbon is attached to the secondary carbon of propane, we obtain isobutane



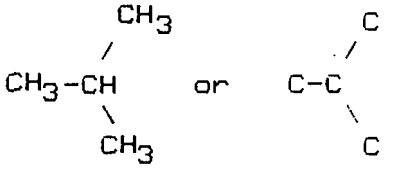
where the center carbon is now a _____ (__°) carbon.

1-12 To write all possible pentanes (5-carbon alkanes) we must look at two isomeric butanes and at the number of different positions in the butanes where a fifth carbon can be attached. There are two different kinds of carbons in n-butane (C-C-C-C). If a fifth carbon is attached at a primary carbon we obtain the skeleton formula:

1-13 If the fifth carbon, however, is attached to a secondary carbon of butane, the skeleton formula of the resulting pentane is:

This substance is called isopentane.

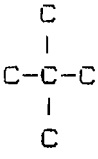
1-14 The second four-carbon molecule, isobutane



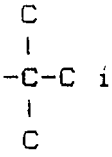
can be seen to have three identical CH_3 groups attached to a central tertiary carbon atom. A fifth carbon can therefore be attached either to an outer primary carbon (replacing an H of one of the CH_3 groups) or to the central carbon. The resulting carbon skeletons are:

1-15 The first of these formuals, you will notice, is identical with the one in section _____ where it is named _____.

1-16 The second formula in the answer to Section 1-14



is a new pentane. Since the prefix neo comes from the Greek neos meaning new, it was attached to the pentane, so that the resulting name



for is _____.

1-17 No pentanes (of formula C_5H_{12}) with skeletons other than the above three have been discovered. And no structural formulas for molecules C_5H_{12} with different skeletons can be devised. Note that the word skeleton is an apt one for our formulas. Just as arms and legs can move without destroying a person, so a skeleton formula can have its atomic positions shifted so long as no bonds are broken. C-C-C refers to the same chemical as the

```
  |
  C
```

formulas

```
    C   C
     \ /
      C
      |
      C
```

and

```
    C
    |
  C-C.
    |
    C
```

The formulas

```
      C
      |
C-C-C-C   and  C-C-C
  |            |
  C            C
```

refer to the (same/different) chemical(s).

1-18 Among the hexanes (6 carbons), neohexane is

```
    C
    |
  C-C-C-C.
    |
    C
```

Neopentane and neohexane both contain one _____ (__') carbon atom. No other pentane or hexane (or smaller molecule) contains anything more complex than a tertiary (3') carbon.

1-19 There are more than three different hexanes, C_6H_{14}. The number of different carbon skeletons for this formula is _____; and the corresponding skeleton structures are:

1-20 If your answer to the previous section was more than 5, you should convince yourself that some of your structures were duplicates - this is, they could be converted into each other simply by turning formulas and bending bonds. Note that ring structures such as C-C-C are excluded because they

```
  | |
C-C-C
```

could not accomodate 14 hydrogen atoms.

What should we call formulas III and V? We have run out of names and the invention of new prefixes is not very helpful for subsequently figuring out formulas. This is the reason chemists finally worked out a SYSTEMATIC naming system in which formulas could be derived from the information given in the name if a few simple rules were memorized. There are 9 heptanes (C_7H_{16}), 18 octanes (C_8H), 35 nonanes (C_9H_{20}), 75 decanes ($C_{10}H$), etc. You may want to convince yourself that some of these numbers are correct. We would need a lot of prefixes to distinguish them.

One final point before we leave common naming. You may have noticed the prefix iso. When a compound has iso preceding it there is this three-carbon fragment, attached from the middle carbon to

```
  C
   \
    C-
   /
  C
```

an unbranched chain of carbon atoms. Isoheptane (molecular) formula C_7H_{16}) should therefore have the skeleton structure:

THE SYSTEMATIC NAMING OF ALKANES

In working through the common names of hydrocarbons we ran out of prefixes after defining the meanings of n-, iso, sec-, tert-, and neo. Now there is no difficulty in thinking up new prefixes; the problem is to remember their meanings. The situation finally became so confused that an international congress was called at Geneva, Switzerland in 1892 to devise a naming system by which not only presently known compounds but also those to be prepared in the future could be given names understandable to anyone trained in the system.

A "Definitive Report of the Commission on the Reform of the Nomenclature of Organic Chemistry" was unanimously adopted by the International Union of Pure and Applied Chemistry (IUPAC). Names based on the international rules are called Systematic names, Geneva names or IUPAC names. The rules, with comments, were published in J. Am. Chem. Soc. 82, 5545-5584 (1960)

2-1 The first rule of the IUPAC sytem is to look for the longest chain of carbon atoms, eliminating all branches off the longest continuous chain. This chain is known as the "parent chain". Branches are named subsequently.

The longest continuous chain in isobutane

is a chain of _____ carbon atoms.
(number)

2-2 Isobutane is therefore considered a derivative of the "parent" three-carbon alkane whose molecular formula is _____; this is called p_____e.

2-3 Before we proceed we should review some earlier information needed in systematic naming:
The two-carbon alkane is called _____.

2-4 The simplest alkane, CH_4 is called _____.

2-5 To convert propane, C_3H ___, to isobutane, C_4H ___, we need to replace one hydrogen atom of propane by a group C__H__ (_____ group).

2-6 If instead we had replaced a hydrogen atom in propane, C_3H_8, by a two-carbon group, in order to form a new alkane, C_5H_{12}, that group would have had the formula _____.

2-7 A one-carbon group that can replace a hydrogen atom has the formula CH_3; and a two carbon group, C_2H_5. An n-carbon group that can replace a hydrogen atom should then have the formula C_nH_____.

2-8 We say that the group CH_3 is derived from CH_4 by removing one hydrogen atom; since CH_4 is methane, CH_3 is called methyl. Since C_2H_6 is ethane, C_2H_5 is called _____. (In general, we replace the ending -ane by -yl.

2-9 Methyl, ethyl, propyl, etc. are called alkyl groups. Thus, C_4H_9 is called _____ and is an example of an _____ group.

2-10 C_3H_8 is _____; and C_3H_7 is _____.

2-11 Now we can return to the systematic naming of isobutane. Its molecular formula is C_4H_{10}. Its carbon "skeleton" looks like this:

```
C-C-C
    |
    C
```

Its longest unbranched carbon chain contains three carbon atoms. The name of the three-carbon "parent" alkane is _____.

2-12 In addition to the three-carbon chain, isobutane contains a one-carbon group attached to the middle carbon. This one-carbon group has the formula _____ and is called a _____ group.

2-13 Isobutane, therefore, has the IUPAC name methyl-propane. More precisely it is named 2-methylpropane. Except in the simplest cases, the point of attachement of any branch must be specified. Thus there are two methylpentanes:

```
1 2 3 4 5          5 4 3 2 1          1 2 3 4 5
C-C-C-C-C          C-C-C-C-C          C-C-C-C-C
  |          =           |                |
  C                      C                C
```

2-methylpentane 3-methylpentane

We number the longest or "parent" chain, beginning at the end that makes the point of attachment occur at the smallest possible number. Since a six-carbon hydrocarbon is named hexane (prefixes such as n- are not used in the IUPAC system), the Systematic name for

```
    C
    |
C-C-C-C-C-C
```

must be _____ .

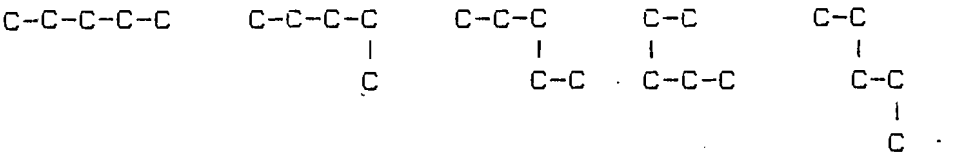
2-14 The compound with the structural formula

```
    H H H H H H H
    | | | | | | |
H-C-C-C-C-C-C-C-H
    | | | | | | |
    H H H H H H H
```

is heptane. To simplify formula writing, the heptane formula is often written simply as $CH_3CH_2CH_2CH_2CH_2CH_2CH_3$ or even as $CH_3(CH_2)_5CH_3$. Such formulas are spoken of as "condensed formulas". Similarly the formula of pentane (five carbons) may be written in condensed form as

_____ or _____

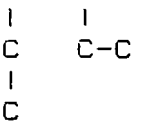
2-15 Note that a five-carbon chain need not be written on a horizontal line. The following carbon skeletons all represent pentane



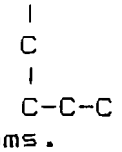
Remember that two different formulas represent the same chemical compound if one formula can be converted into the other simply by twisting the formula but without breaking any bonds. By contrast, C-C-C-C-C can only be converted into C-C-C-C if at

least one C-C bond and one C-H bond are broken. Thus C-C-C-C is a methylbutane because the longest

continuous chain contains four carbon atoms. On the

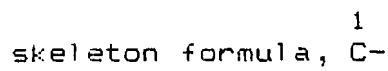
other hand C-C-C-C is hexane.  is _____.

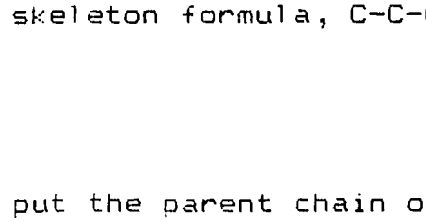
2-16 The "parent" chain or longest continuous chain of carbon atoms (not necessarily) in a straight line) in the carbon skeleton C-C-C-C-C contains



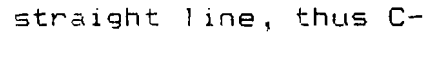
_____ carbon atoms.
(number)

2-17 For convenience in naming, let us rewrite our



skeleton formula,  in such a way as to

put the parent chain of seven carbon atoms in a



straight line, thus

You should make quite sure that this can be done without the breaking of any bonds. The molecule is now seen to be a substituted heptane. To the parent heptane chain is attached one branch of _____ carbon atoms. This branch, C_2H_5, is an _____ group.

2-18

```
C-C-C-C-C-C-C
    |
    C
    |
    C
```

Numbering the parent chain from that end which makes the branch number the smallest possible, leads to position number _____ for the branch.

2-19

```
C-C-C-C-C-C-C
    |
    C
    |
    C
```

OR

```
C-C-C-C-C
    |
    C
    |
    C-C-C
```

is 3-ethylheptane.

The condensed formula $(CH_3CH_2)_3CH$ can be expanded to

```
          H H H H H
          | | | | |
H-C-C-C-C-C-H
| | | | |
H H | H H
    |
  H-C-H
    |
  H-C-H
    |
    H
```

. Its name must be _____.

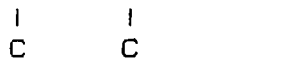
2-20 The first ten unbranched alkanes have the IUPAC names and formulas as follows:

methane	CH_4	hexane	C_6H_{14}
ethane	C_2H_6	heptane	C_7H_{16}
propane	C_3H_8	octane	C_8H_{18}
butane	C_4H_{10}	nonane	C_9H_{20}
pentane	C_5H_{12}	decane	$C_{10}H_{22}$

```
C-C-C-C-C-C-C-C-C
          |
          C
          |
          C
          |
          C
```

would be called _____ .

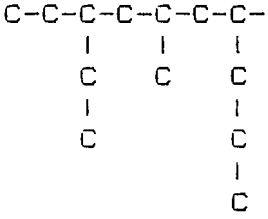
2-21 The formula



is named 3,6-dimethyldecane. 3,6-dimethyl designates that there are two methyl groups attached to the decane chain, one at the third and one at the sixth carbon atom. If both methyls were attached at the same carbon atom of the parent chain, the number designating that carbon would be repeated: 2,2-dimethylpropane has the carbon skeleton:

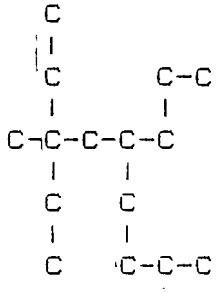
2-22 Three methyl branches are written as trimethyl; four ethyl branches, tetraethyl. 3,3,5-triethyloctane has the carbon skeleton:

2-23 If several groups appear as branches, they are usually listed in alphabetical order of alkyl groups and it is this practice we shall follow. Thus,



is named 3-ethyl-5-methyl-7-propyldecane. The carbon skeleton for 5-butyl-4-methylnonane is:

2-24 What is the name of



(Remember to locate the longest continuous chain first - and that it does not have to be in a straight line in the formula. Name substituent groups in alphabetical order. Remember, too, that numbering is started from that end which gives the first branch encountered the smaller number, regardless of the size of the branch.)

2-25 Name the following: (write out the expanded skeletons for these formulas before naming unless you are quite sure what they represent)

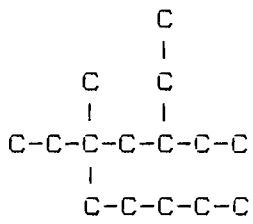
(a) $CH_3(CH_2)_7CH_3$ _____

(b) $(CH_3CH_2)_4C$ _____

2-26 2-methyl-4,5-dipropyloctane has the skeleton structure:

(Note that methyl precedes dipropyl in the name, because only the names of alkyl groups are considered for alphabetical ordering. Prefixes di-, tri-, tetra-, are attached after the order of the groups is established.

2-27 What is the IUPAC name for



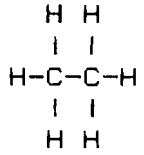
_____

2-28 The name for C-C-C-C-C (with a C branch on the second C) is _____

2-29 The skeleton structure of 3,3,5-triethylheptane is:

THE SYSTEMATIC NAMING OF ALKENES, ALKYNES, DIENES, AND SIMPLE CYCLIC HYDROCARBONS

3-1 The molecules we have discussed so far have pairs of atoms linked by single bonds only. Ethane, for instance, has the structural formula



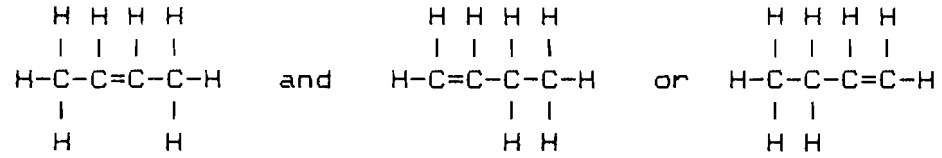
Suppose, however, that two carbon atoms were linked to each other by a pair of bonds, thus C=C. Then, since carbon has a valence of four, only two other atoms can be linked by each carbon. The simplest hydrocarbon containing a double bond, therefore, has the molecular formula C_2H_4 and the structural formula:

3-2 The substance of molecular formula C_2H_4 is commonly known as ethylene. Its systematic name is ethene. Hydrocarbons containing one double bond are known as **alkenes.** Alkenes may be thought of as being derived from alkanes by the removal of a pair of hydrogen atoms from adjacent carbons. These adjacent carbons become doubly linked. In naming an alkene, we first name the alkane with the same number of carbon atoms and then replace the ending ane by ene. Since C_3H_8 is named propane, the name of the compound with formula C_3H_6 should be _____.

3-3 Since alkanes have the general formula C_nH_{2n+2}, and alkenes are derived from them by the loss of two hydrogen atoms, the general formula for alkenes is _____.

3-4 The molecular formula for ethene is C_2H_4. For the three-carbon alkene, propene, it is C_3H_6. For a five carbon alkene the molecular formula must be _____ .

3-5 In converting butane, $CH_3CH_2CH_2CH_3$, to an alkene, two different structures can be formed. The pair of hydrogens may be lost either from the the two middle carbons or from a middle and the adjacent end carbons. The resulting butenes have the formulas and names:



2-butene 1-butene

The number of different positions for a double bond in a five-carbon chain must be _____.

3-6 The number of different positions for a double bond in a six-carbon chain must be _____.

3-7 In section 3-5 we gave the name of $CH_2=CH-CH_2-CH_3$ as 1-butene and of $CH_3CH=CH-CH_3$ as 2-butene. The IUPAC rule is to number the longest continuous chain of carbons that contains the double bond from the end that places the double bond at the lowest numbered carbons. According to this rule the double bond in the hexene $CH_3-CH_2-CH_2CH=CH-CH_3$ occurs between carbon atoms _____ and _____.

3-8 Since double bonds always occur between adjacent carbons, it is superfluous to indicate the numbers of both carbons terminating the double bond. It is enough to indicate the lower number. Thus, 2-hexene has the formula $CH_3-CH=CH-CH_2-CH_2CH_3$. The formula for 3-hexene, written in the same form (a condensed structural formula) would be

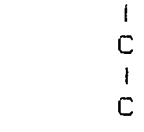
3-9 The name for $CH_3-CH=CH-CH_2-CH_2CH_2CH_3$ is _____.

3-10 When branches occur, we look for the longest carbon chain of which the double bond is a part (this is the "parent" alkene here).
Thus $CH_2=C(CH_2CH_3)-CH_2-CH_3$ will be named as a substituted pentene, not a substituted hexane. Its name is 2-ethyl-1-pentene. The parent alkene in the formula $CH_2=C(CH_2CH_3)-CH_3$ is _____.

3-11 The systematic name of $CH_2=C(CH_2CH_3)-CH_3$ is therefore _____.

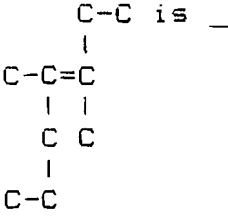
3-12 Note that the numbering is determined by the location of the double bond only, and not by the position of the branches. Thus $(CH_3)_2CHCH_2CH_2CH_2CH_2CH=CH_2$ is 7-methyl-1-octene (not 2-methyl-7-octene). Accordingly, $(CH_3)_2CH-CH=CH-CH_3$ is named _____.

3-13 The name of the alkene whose carbon skeleton is



must be _____.

3-14 The name for



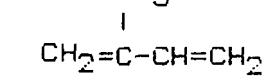
is _____.

3-15 The carbon skeleton of the substance 2-methyl-6-propyl-4-nonene may be written:

3-16 **Polyenes-Hydrocarbons with two or more double bonds**

$CH_2=CH-CH=CH_2$ is named 1,3-butadiene. The ending for a molecule with three double bonds is -atriene, with four -atetraene, and so on. $CH_2=CH-CH=CH-CH=CH_2$ is accordingly named _____.

3-17 In branched hydrocarbon polyenes, the longest carbon chain containing the double bonds is numbered and named first; the branches are then numbered and named, and written preceding the parent name. "Isoprene", the "building block" of natural rubber has the formula



Its systematic name is 2-methyl-1,3-butadiene. The formula for 2,3-dimethyl-2,4,5-octatriene is:

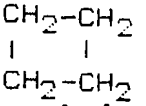
3-18 **Alkynes** (pronounced to rhyme with lines). An alkyne contains a triple bond C=C. Polyynes contain two or more such bonds. The rules for naming follow those described for alkenes. The simplest alkyne has the molecular formula _____.

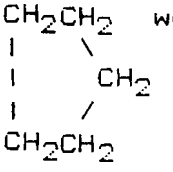
3-19 The systematic name of the substance whose molecular formula is C_2H_2 is ethyne. Its more commone name is acetylene. The structural formula for ethyne is:

3-20 The general molecular formula for alkynes is C_nH_{2n-2}. The molecular formula for 3-octyne will therefore be _____.

3-21 The condensed structural formula for 3-octyne is:

3-22 **Cyclic Hydrocarbons**

To form a ring from a carbon chain involves the removal of two hydrogen atoms from non-adjacent carbon atoms and the linking of the carbons thus exposed. Cyclobutane is  Thus, cycloalkanes have the general formula C_nH_{2n} (as do alkenes). The molecular formula of cyclopropane, therefore, is _____, and its structural formula is:

3-23 The name for  would be _____.

3-24 Since cycloalkanes have the formula C_nH_{2n}, cycloalkenes (one double bond) have the formula C_nH_{2n-2}. Cyclohexene, therefore, has the formula C_6H____. Its structural formula is:

3-25 1,3-cyclohexadiene has the structural formula:

3-26 Benzene, C_6H_6, has the name 1,3,5-cyclohexatriene. The structural formula for benzene is:

3-27 The stuctural diagram for 3,4 -dimethylcyclopentene is:

3-28 The structural diagram for 5-ethyl-5,6-dimethyl-1,3-cycloheptadiene is:

THE SYSTEMATIC NAMING OF ALKYL HALIDES

ORG.NOM.2

4-1 When a halogen atom is introduced into a hydrocarbon molecule, naming proceeds as if the halogen were simply a branch. The hydrocarbon is named as if the halogen were absent; the nature and position of the halogen is then indicated. The hydrocarbon from which $CH_3CH_2\underset{\displaystyle Cl}{\underset{|}{C}}HCH_2CH_3$ is derived is called _____.

4-2 $CH_3CH_2\underset{\displaystyle Cl}{\underset{|}{C}}HCH_2CH_3$ is called 3-chloropentane. Analogously, $CH_3CH_2CH_2Cl$ must be named _____.

4-3 A Cl substituent is referred to as chloro-; Br substituents should be named _____.

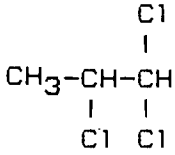
4-4 CH_3CHFCH_3 is 2-fluoropropane. If I is called iodo-, $CH_3CH_2CH_2CHICH_2CH_3$ should be named _____.

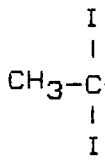
4-5 The name of the hydrocarbon from which $CH_3-\underset{\displaystyle CH_3}{\underset{|}{C}}H-CH_2-\underset{\displaystyle Br}{\underset{|}{C}}H-\underset{\displaystyle CH_3}{\underset{|}{C}}H-CH_3$ is derived is

_____.

4-6 $(CH_3)_2CHCH_2\ CHBrCH(CH_3)_2$ is named 3-bromo-2,5-dimethylhexane. (This is the same substance as shown in 4-5). Substituents are listed in alphabetical order, regardless of their nature. $CH_3CH_2CHClCH_2\underset{\displaystyle CH_3}{\underset{|}{C}}HCH_3$ is _____.

4-7 If there are two or more atoms of the same halogen present, the prefixes di-, tri-, tetra-, etc. are used. 1,1,2-trichloropropane is

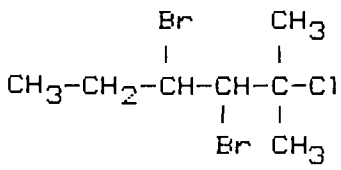




is _____ .

4-8 $ICH_2-CI_2-CH_2I$ is _____.

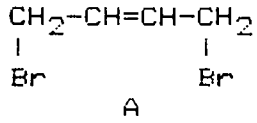
4-9



is _____.

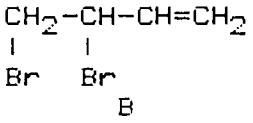
4-10 If double bonds are present, the hydrocarbon is still named as if the halogen were absent. The halogen is named subsequently and the name is added to the hydrocarbon name. $F-CH=CH-CH_2-CH_3$ is 1-fluoro-1-butene. $CH_3-CH=CH-CH_2I$ is _____.

4-11 1,3 butadiene $CH_2=CH-CH=CH_2$ on bromination yields



A

and

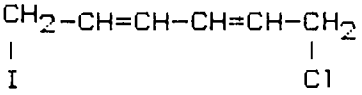


B

Compound A would be named _____

and B _____

4-12



named

_____.

THE SYSTEMATIC NAMING OF ALCOHOLS

5-1 If a hydrocarbon is characterized by the general formula R-H, an alcohol has the general formula R-OH. The alcohol whose parent hydrocarbon is ethane, C_2H_6, has the formula _____.

5-2 Halogen compounds were considered substitution products of hydrocarbons. Alcohols, on the other hand, are considered functional derivatives. The "functional group" OH is considered an integral part of the molecular structure for naming purposes:

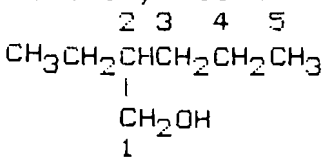
C_2H_6 ethane C_2H_5OH ethanol
$CH_3CH_2CH_2CH_2CH_3$ pentane
$CH_3CH_2CH_2CH(OH)CH_3$ 2-pentanol
$CH_3CH_2CH_3$ propane
$CH_3CH_2CH_2OH$ _____. (include position number)

5-3 $CH_3CH_2CH_2CH_3$ $CH_3CH_2CH_2CH_2OH$

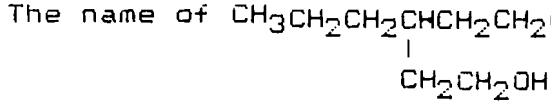
butane _____

5-4 $CH_3(CH_2)_7OH$ is named _____.

5-5 Naming proceeds as for alkanes with one exception. Instead of looking for the longest carbon chain, we seek the longest carbon chain to which the OH group is directly attached.



is 2-ethyl-1-pentanol (Note that it is not considered as a substituted hexane.)

The name of  is

_____.

5-6 Note that numbering on the parent alcohol chain is determined by the OH group. Its location is given the smallest possible number.

$CH_3CH_2CHCH_3$ is 2-butanol not 3-butanol
|
OH

$CH_3CH_2CH_2CH(OH)CH_2CH_3$ is _____.

5-7 Once the numbering system is determined by the location of the OH group, other branches, alkyl or halogen are named in the usual way.

$CH_3-CH_2-C(CH_3)(CH_3)-OH$ is named _____.

5-8

$CH_3CCH_2CH_2C(CH_2CH_3)(CHCH_3)-CH_3$ is _____.
| |
CH_3 OH

5-9 POLYHYDROXY COMPOUNDS

If possible, that carbon chain is chosen to which all OH groups are directly attached.

CH_2OH-CH_2OH is 1,2-ethanediol

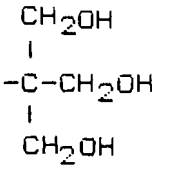
(common name is ethylene glycol, (antifreeze))

$CH_3CH_2-C(CH_2OH)(CH_2OH)-OH$ is _____.

5-10 2,2-dimethyl-1,3-propanediol has the structural formula:

5-11 The insect repellent "6-12" (2-ethyl-1,3-hexanediol) has the structural formula:

5-12 If it is impossible to find a continuous carbon chain to which all OH groups are attached, that chain is chosen to which most OH groups are attached. The remaining groups are named as hydroxy substituents.

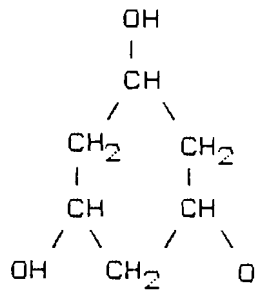


$CH_3-C(CH_2OH)_2-CH_2OH$ is 2-(hydroxymethyl)-2-methyl-1,3-propanediol

4-(hydroxymethyl)-1,6-heptanediol has the formula

5-13 1,2-cyclopentanediol has the formula:

5-14



is _____.

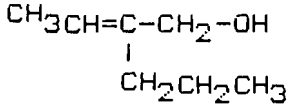
5-15 <u>UNSATURATED ALCOHOLS</u>

$CH_3CH=CH-CH_2OH$ is 2-buten-1-ol

$CH_2=CH-CH_2OH$ is 2-propen-1-ol (note OH (allyl alcohol) group takes precedence in numbering)

3-buten-2-ol has the formula:

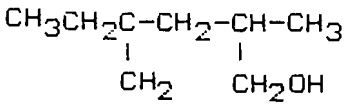
5-16 If there is a choice of chains, the most unsaturated is chosen as long as it still contains the OH group (i.e., we line up again the maximum number of functional groups on the parent chain).



is _____.

5-17 Remembering that compounds with triple bonds are called alkynes, 2-propyn-1-ol has the formula:

5-18

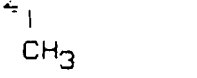


is _____.

5-19 The formula of 2,2,5-trimethyl-3-hexene-1,5-diol is:

THE SYSTEMATIC NAMING OF ALDEHYDES AND KETONES

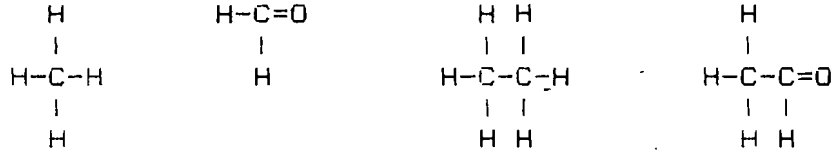
6-1 Aldehydes and ketones may be considered as derived from hydrocarbons by replacing one CH_2 group by a carbonyl group C=O. If the C=O group is at the end of a chain or branch we have an aldehyde, if flanked by a carbon on each side, a ketone. Which of the following (A,B,C,etc.) are aldehydes?

(A) $CH_3HC{=}O$ (B) 

(C) $(CH_3)_2CHCOCH(CH_3)_2$ (D) $HCHO$

(E) CH_3COCH_3 (F) $HCOC_2H_5$

6-2

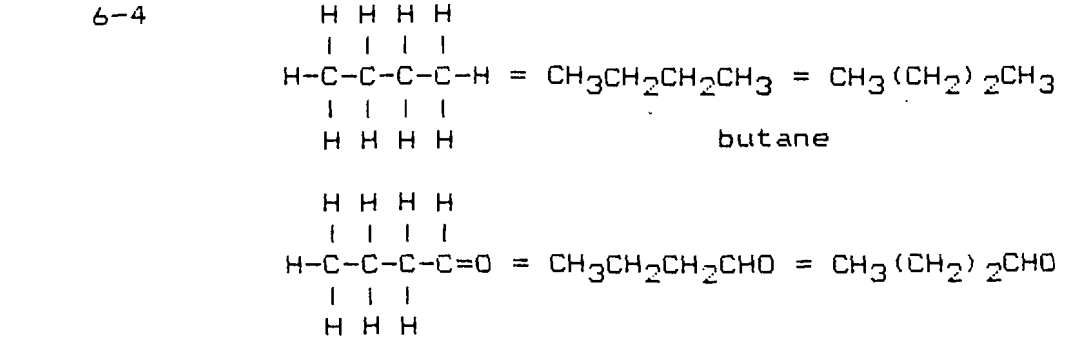


Methane Methanal Ethane _____

Note: No position number is needed, because CHO group is always considered as position 1.

6-3 propane $CH_3CH_2CH_3$ propanal

6-4



$CH_3CH_2CH_2CH_3 = CH_3(CH_2)_2CH_3$ butane

$CH_3CH_2CH_2CHO = CH_3(CH_2)_2CHO$

6-5 $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CHO$

The name is _____.

6-6 CH_3CH_2CHCHO is 2-methylbutanal
CH_3

$CH_3CH_2CHCH_2CHO$
C_2H_5 is _____.

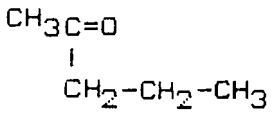
6-7 The structural diagram for 2-chloropropanal is:

6-8 2,2,2-trichloroethanal:

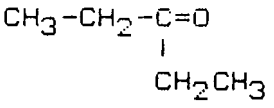
6-9 $CH_3-C(=O)-CH_3$ propanone - a ketone
common name acetone

$CH_3-C(=O)-CH_2CH_3$ _____

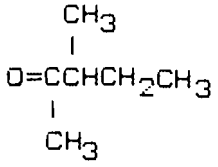
(Note: No location number is needed as the name is unambiguous)

6-10 

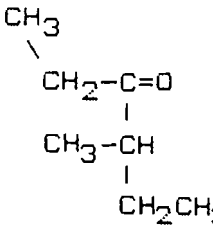
2-pentanone



_____

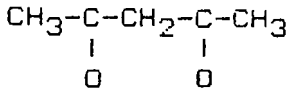
6-11 

_____.

6-12 

Note:look for the longest chain containing the C=O group

_____.

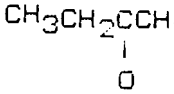
6-13  is 2,4-pentanedione

2,3-hexanedione is:

6-14 1,4-cyclohexanedione is:

6-15 $CH_3CH=CH-CHO$ is 2-butenal

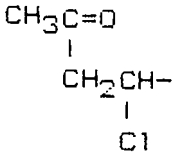
3-penten-2-one is:

6-16 C=O takes precedence over OH in determining the parent name thus: 

1-hydroxy-3-pentanone, and 3-hydroxypentanal is:

6-17 5-chloro-3-heptanal is:

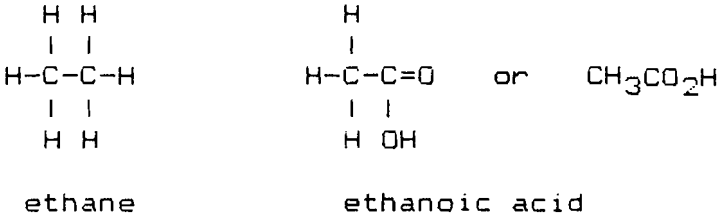
Names and Structures of Organic Compounds - Page 28

6-18  is _____.

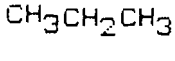
6-19 2,5-cyclohexadien-1-one has the structural formula:

6-20 2,5-heptadien-4-one has the structural formula:

THE SYSTEMATIC NAMING OF CARBOXYLIC ACIDS

7-1 

ethane ethanoic acid



propane propanoic acid

7-2 Pentanoic acid is:

7-3 3-hydroxybutanoic acid is

Note: The carbon of the CO_2H group can only be at the end of a carbon chain, never in the middle. Thus it is considered as carbon atom number 1, taking precedence over ketone or alcohol functions.

7-4 2-butenoic acid is:

7-5 "Acrylic acid" has the formula $CH_2=CHCO_2H$. Its systematic name is _____.

7-6 $CH_3CHCH_2CO_2H$ is 3-methylpentanoic acid
CH_3CH_2

$(CH_3CH_2)_3CCO_2H$ is _____.

7-7 $CH_3-CH_2-CH(CO_2H)-CH_2-CH_3$ is _____.

7-8 3-5-hexadienoic acid is:

7-9 CH_2CO_2H
CH_2CO_2H is butanedioic acid

$CH_2(CO_2H)_2$ is _____.

7-10 3-hydroxypentanoic acid is:

THE SYSTEMATIC NAMING OF ESTERS

8-1 An ester can usually be decomposed by water (catalyzed in most cases by acids and bases) to form an alcohol and a carboxylic acid. The names of esters reflect this relationship. Thus an ester which on hydrolysis forms 1-propanol and ethanoic acid is named propyl ethanoate. Ethyl butanoate when allowed to react with water would produce

_____ and _____.

8-2 You will notice that the alcohol part of the ester is always named first, and the acid part (containing the C=O group) second. Unfortunately the formulas are usually written with the acid part first. Thus the formula of methyl propanoate is usually written $C_2H_5C(=O)OCH_3$, or $C_2H_5CO_2CH_3$, or $C_2H_5COOCH_3$

Our problem then is to unscramble the formula to be sure which part belongs to the acid and which to the alcohol. Let us look at the equation for an ester synthesis:

$$R\text{-}C(=O)\text{-}O\text{-}H + R^1\text{-}O\text{-}H \xrightarrow[\text{catalysis}]{\text{acid}} R\text{-}C(=O)\text{-}O\text{-}R^1 + H_2O$$

Note that there is a difference in the bonding of the R and R^1 groups. The R group throughout the reaction is attached to a(n) _____ atom, whereas R^1 in alcohol and ester is attached to a(n) _____ atom.

8-3 In the ester formula, then, the alkyl group attached to carbon belongs to the acid portion, whereas the alkyl group attached to oxygen came from the alcohol. If we unscramble the formula $CH_3CO_2C_2H_5$ to show all bonds, we obtain the structural formula:

8-4 We may write the formulas of the acid and the alcohol from which this ester $CH_3CO_2C_2H_5$ was derived. The formula of the acid was

and of the alcohol

8-5 The IUPAC names of these two substances are

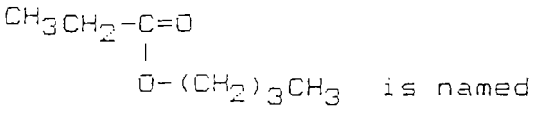
_____ and _____.

8-6 The name of the ester obtained from these two substances is therefore _____.

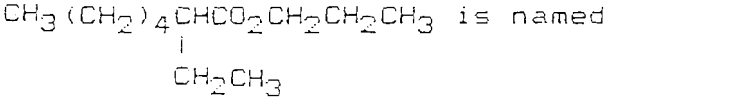
8-7 The name of $CH_3CH_2CH_2CO_2CH_3$ is

_____.

8-8 If the constituent alcohol is 1-pentanol and the acid is 2-methylhexanoic acid the ester will be named pentyl 2-methylhexanoate. Its formula must be

8-9  is named

_____.

8-10  is named

_____.